Supervised Learning

Filter Methods

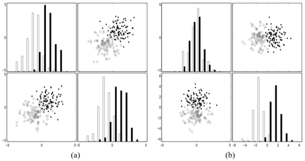
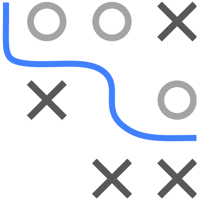


Figure 1: **Information gain from presumably redundant variables.** (a) A two class problem with independently and identically distributed (i.i.d.) variables. Each class has a Gaussian distribution with no covariance. (b) The same example after a 45 degree rotation showing that a combination of the two variables yields a separation improvement by a factor $\sqrt{2}$. I.i.d. variables are not truly redundant.

Learning goals

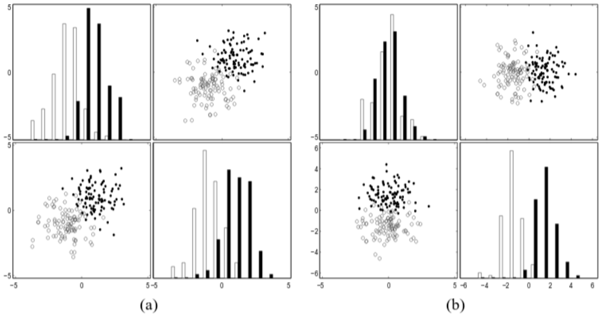
- Understand how filter methods work
- Understand how to apply them for feature selection
- Understand advantages and disadvantages, and how to overcome them.

INTRODUCTION



- Mostly, **filter methods** construct a measure that describes the strength of the (univariate) dependency between a feature and the target variable.
- Typically, this yields a numeric score for each feature *j*. That is what is known as **variable-ranking**.
- Filters are in general independent of a specific classification learner and can be applied generically.
- Filter methods are strongly related to methods for determining variable importance.

EXAMPLES, TAKEN FROM GUYON (2003)



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Isabelle Guyon, André Elisseeff (2003). An Introduction to Variable and Feature Selection. Journal of Machine Learning Research (3) p. 1157-1182.

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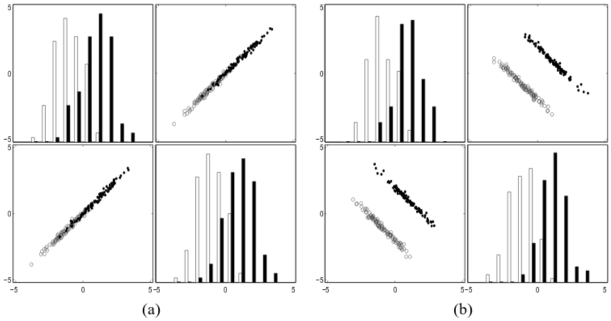

Figure 2: **Intra-class covariance.** In projection on the axes, the distributions of the two variables are the same as in the previous example. (a) The class conditional distributions have a high covariance in the direction of the line of the two class centers. There is no significant gain in separation by using two variables instead of just one. (b) The class conditional distributions have a high covariance in the direction perpendicular to the line of the two class centers. An important separation gain is obtained by using two variables instead of one.

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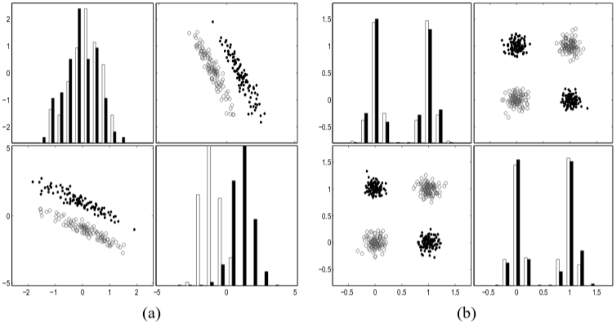

Figure 3: **A variable useless by itself can be useful together with others.** (a) One variable has completely overlapping class conditional densities. Still, using it jointly with the other variable improves class separability compared to using the other variable alone. (b) XOR-like or chessboard-like problems. The classes consist of disjoint clumps such that in projection on the axes the class conditional densities overlap perfectly. Therefore, individual variables have no separation power. Still, taken together, the variables provide good class separability .

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FILTER: χ^2-STATISTIC

- Test for independence between the j-th feature and the target y.
- Numeric features or targets need to be discretized.
- Hypotheses:

  $$\begin{aligned} H_0 &: p(x_j = l, y = k) = p(x_j = l)\, p(y = k), \forall j = 1, \dots, k_1 \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad \forall k = 1, \dots, k_2 \\ H_1 &: \exists\, j, k : p(x_j = l, y = k) \neq p(x_j = l)\, p(y = k) \end{aligned}$$

- Calculate the χ^2-statistic for each feature-target combination:

  $$\chi^2 = \sum_{j=1}^{k_1} \sum_{k=1}^{k_2} \left(\frac{e_{jk} - \tilde{e}_{jk}}{\tilde{e}_{jk}}\right) \quad \underset{approx.}{\overset{H_0}{\sim}} \quad \chi^2((k_1 - 1)(k_2 - 1))$$

  where e_{jk} is the observed relative frequency of pair (j, k) and $\tilde{e}_{jk} = \frac{e_{j.} e_{.k}}{n}$ is the expected relative frequency.
- The greater χ^2, the more dependent is the feature-target combination, the more relevant is the feature.

FILTER: PEARSON & SPEARMAN CORRELATION

Pearson correlation $r(\mathbf{x}_j, y)$**:**

- For numeric features and targets only.
- Most sensitive for linear or monotonic relationships.
- $r(\mathbf{x}_j, y) = \frac{\sum_{i=1}^{n}(x_j^{(i)} - \bar{x}_j)(y^{(i)} - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_j^{(i)} - \bar{x}_j)}\sqrt{(\sum_{i=1}^{n} y^{(i)} - \bar{y})}}, \qquad -1 \leq r \leq 1$

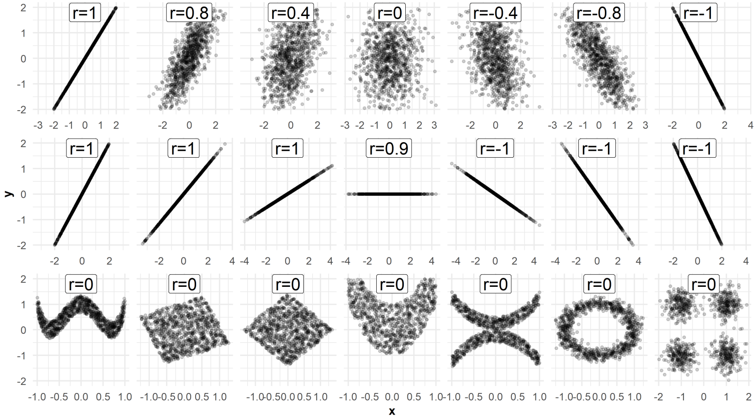
Spearman correlation $r_{SP}(\mathbf{x}_j, y)$**:**

- For features and targets at least on an ordinal scale.
- Equivalent to Pearson correlation computed on the ranks.
- Assesses monotonicity of the dependency relationship.

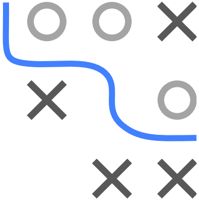
Use absolute values $|r(\mathbf{x}_j, y)|$ for feature ranking: higher score indicates a higher relevance.

FILTER: PEARSON & SPEARMAN CORRELATION

Only **linear** dependency structure, non-linear (non-monotonic) aspects are not captured by *r*:



FILTER: DISTANCE CORRELATION

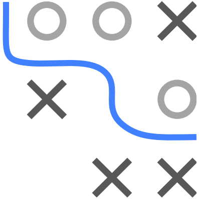


$$r_D(\mathbf{x}_j, y) = \sqrt{\frac{c_D^2(\mathbf{x}_j, y)}{\sqrt{c_D^2(\mathbf{x}_j, \mathbf{x}_j) c_D^2(y, y)}}} :$$

Normed version of **distance covariance**
$c_D(\mathbf{x}_j, y) = \frac{1}{n^2} \sum_{i=1}^n \sum_{k=1}^n D_{\mathbf{x}_j}^{(ik)} D_y^{(ik)}$ for

- distances of observations: $d\left(x_j^{(i)}, x_j^{(k)}\right)$,
- mean distances $\bar{d}_{xj}^{(i\cdot)} = \frac{1}{n} \sum_{k=1}^n d\left(x_j^{(i)}, x_j^{(k)}\right)$,
- and centered pairwise distances
  $D_x^{(ik)} = d\left(x_j^{(i)}, x_j^{(k)}\right) - (\bar{d}_{xj}^{(i\cdot)} + \bar{d}_{xj}^{(\cdot k)} - \bar{d}_{xj}^{(\cdot\cdot)})$

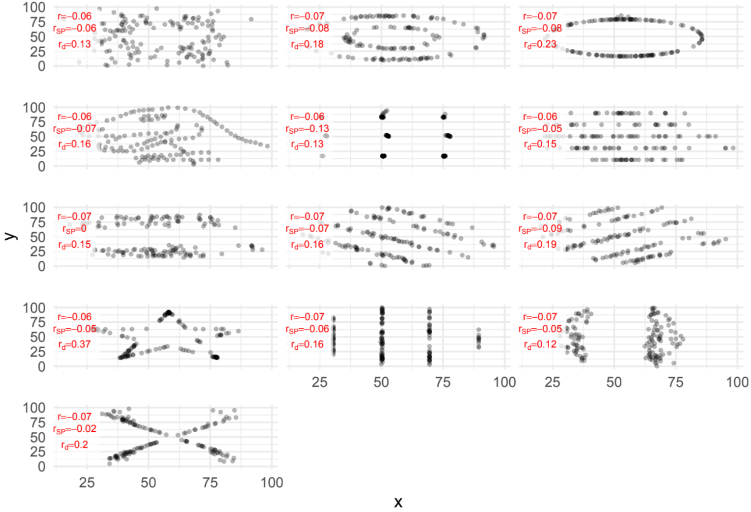
FILTER: DISTANCE CORRELATION



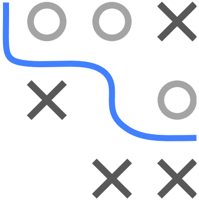
Properties:

- $0 \leq r_D(\mathbf{x}_j, y) \leq 1 \quad \forall j \in \{1, \dots, p\}$
- $r_D(\mathbf{x}_j, y) = 0$ only if $\mathbf{x}$ and y are empirically independent (!)
- $r_D(\mathbf{x}_j, y) = 1$ for exact linear dependencies
- also assesses strength of **non-monotonic**, **non-linear** dependencies
- very generally applicable since it only requires distance measures on $\mathcal{X}$ and $\mathcal{Y}$: can also be used for ranking multivariate features, feature combinations or non-tabular inputs (text, images, audio, etc.)
- expensive to compute for large data (i.e., use a subsample)

FILTER: DISTANCE CORRELATION



FILTER: WELCH'S t-TEST

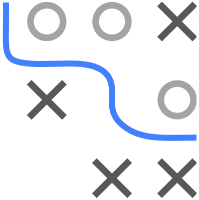


- For binary classification with numeric features.
- Test for unequal means of the j-th feature.
- For notational purposes let $\mathcal{Y} \in \{0, 1\}$. Then the subscript j_0 refers to the j-th feature where $y = 0$ and j_1 where $y = 1$.
- Hypotheses:
  H_0: $\mu_{j_0} = \mu_{j_1}$ vs. H_1: $\mu_{j_0} \neq \mu_{j_1}$
- Calculate Welch's t-statistic for every feature $\mathbf{x}_j$

$$t_j = \frac{\bar{x}_{j_0} - \bar{x}_{j_1}}{\sqrt{\left(\frac{S^2_{x_{j_0}}}{n_0} + \frac{S^2_{x_{j_1}}}{n_1}\right)}}$$

  where $\bar{x}_{j_0}$, $S^2_{x_{j_0}}$ and n_0 are the sample mean, the population variance and the sample size for y = 0, respectively.
- A higher t-score indicates higher relevance of the feature.

FILTER: F-TEST



- For multiclass classification ($g \geq 2$) and numeric features.
- Assesses whether the expected values of a feature $\mathbf{x}_j$ within the classes of the target differ from each other.
- Hypotheses:
  $H_0 : \mu_{j_0} = \mu_{j_1} = \cdots = \mu_{j_g}$ vs. $H_1 : \exists\, k, l : \mu_{j_k} \neq \mu_{j_l}$
- Calculate the F-statistic for each feature-target combination:

$$F = \frac{\text{between-group variability}}{\text{within-group variability}}$$

$$F = \frac{\sum_{k=1}^{g} n_k (\bar{x}_{j_k} - \bar{x}_j)^2 / (g-1)}{\sum_{k=1}^{g} \sum_{i=1}^{n_k} (x_{j_k}^{(i)} - \bar{x}_{j_k})^2 / (n-g)}$$

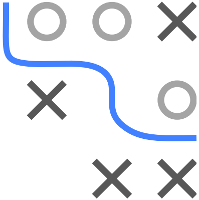
  where $\bar{x}_{j_k}$ is the sample mean of feature $\mathbf{x}_j$ where $y = k$ and $\bar{x}_j$ is the overall sample mean of feature $\mathbf{x}_j$.
- A higher F-score indicates higher relevance of the feature.

FILTER: MUTUAL INFORMATION

$$I(X;Y) = \mathbb{E}_{p(x,y)}\left[\log \frac{p(X,Y)}{p(X)p(Y)}\right]$$

- Each variable $\mathbf{x}_j$ is rated according to $I(\mathbf{x}_j; y)$, this is sometimes called information gain.
- MI is a measure of the amount of "dependence" between variables. It is zero if and only if the variables are independent.
- On the other hand, if one of the variables is a deterministic function of the other, the mutual information is maximal.
- Unlike (Pearson) correlation, mutual information is not limited to real-valued random variables.
- Mutual information can be seen as a more general measure of dependence between variables than correlation.

FILTER



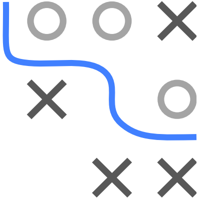
How to combine a filter with a model:

- Calculate filter-values.
- Sort features by value.
- Train model on $\tilde{p}$ best features.

How to choose $\tilde{p}$:

- It can be prescribed by the application.
- Eyeball estimation: Read from filter plots (i.e., Scree plots).
- Use resampling.

FILTER



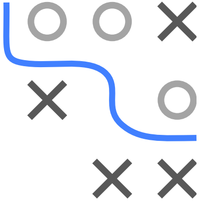
Advantages:

- Easy to calculate.
- Typically scales well with the number of features *p*.
- Mostly interpretable intuitively.
- Combination with every model possible.

Disadvantages:

- Often univariate (not always) ignores multivariate dependencies.
- Redundant features will have similar weights.
- Ignores the learning algorithm.

MINIMUM REDUNDANCY MAXIMUM RELEVANCY



- Most filter type methods select top-ranked features based on a certain filter method (χ^2, rank-correlation, t-test,...) without considering relationships among the features.
- Problems:
  - Features may be correlated and hence, may cause redundancy.
  - Selected features cover narrow regions in space.
- Goal: In addition to maximum relevancy of the features we want the features to be maximally dissimilar to each other (minimum redundancy).
- Features can be either continuous or categorical.

mRMR: CRITERION FUNCTIONS

- Let $S \subset \{1, \dots, p\}$ be a subset of features we want to find.
- Minimize redundancy

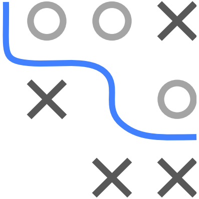
$$\min \operatorname{Red}(S), \qquad \operatorname{Red}(S) = \frac{1}{|S|^2} \sum_{j,l \in S} I_{xx}(\mathbf{x}_j, \mathbf{x}_l)$$

- Maximize relevancy

$$\max \operatorname{Rel}(S), \qquad \operatorname{Rel}(S) = \frac{1}{|S|} \sum_{j \in S} I_{xy}(\mathbf{x}_j, \left\{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(n)}\right\})$$

- I_{xx} measures the strength of the dependency between two features.
- I_{xy} measures the strength of the dependency between a feature and the target.

mRMR: CRITERION FUNCTIONS



- Examples for I_{xx}:
  - Two discrete features: mutual information $I(\mathbf{x}_j, \mathbf{x}_l)$
  - Two numeric features: correlation $|r(\mathbf{x}_j, \mathbf{x}_l)|$

- Examples for I_{xy}:
  - Discrete feature, discrete target: mutual information $I(\mathbf{x}_j, \{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(n)}\})$
  - Continuous feature, discrete target: F-statistic $F(\mathbf{x}_j, \{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(n)}\})$

mRMR: CRITERION FUNCTIONS

- The mRMR feature set is obtained by optimizing the relevancy and the redundancy criterion simultaneously.
- This requires combining the criteria into a single objective function:

$$\Psi(S) = (\mathrm{Rel}(S) - \mathrm{Red}(S)) \quad \text{or} \quad \Psi(S) = (\mathrm{Rel}(S)/\mathrm{Red}(S))$$

- Exact solution requires $\mathcal{O}(|\mathcal{X}|^{|S|})$ searches, where $|\mathcal{X}|$ is the number of features in the whole feature set and $|S|$ is the number of features selected.

In practice, incremental search methods are used to find near-optimal feature sets defined by Ψ:

- Suppose we already have a feature set with $m-1$ features S_{m-1}.

mRMR: CRITERION FUNCTIONS

- Next, we select the m-th feature from the set $\bar{S}_{m-1}$ by selecting the feature that maximizes:

$$\max_{j \in \bar{S}_{m-1}} \left[I_{xy}\left(\mathbf{x}_j, \left\{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(n)}\right\}\right) - \frac{1}{|S_{m-1}|} \sum_{l \in S_{m-1}} I_{xx}(\mathbf{x}_j, \mathbf{x}_l) \right]$$

- The complexity of this incremental algorithm is $\mathcal{O}(|p| \cdot |S|)$.

mRMR: ALGORITHM

Algorithm mRMR algorithm

```
Set $S = \emptyset$, $R = \{1, \dots, p\}$
Find the feature with maximum relevancy:
    $$j^* := \arg\max_j I_{xy}(\mathbf{x}_j, \left\{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(n)}\right\})$$
Set $S = \{j^*\}$ and update $R \leftarrow R \setminus \{j^*\}$
repeat
    Find feature $\mathbf{x}_j$ that maximizes:
        missingformula
    Update $S \leftarrow S \cup \{j^*\}$ and $R \leftarrow R \setminus \{j^*\}$
until Expected number of features have been obtained or some other constraints are satisfied.
```